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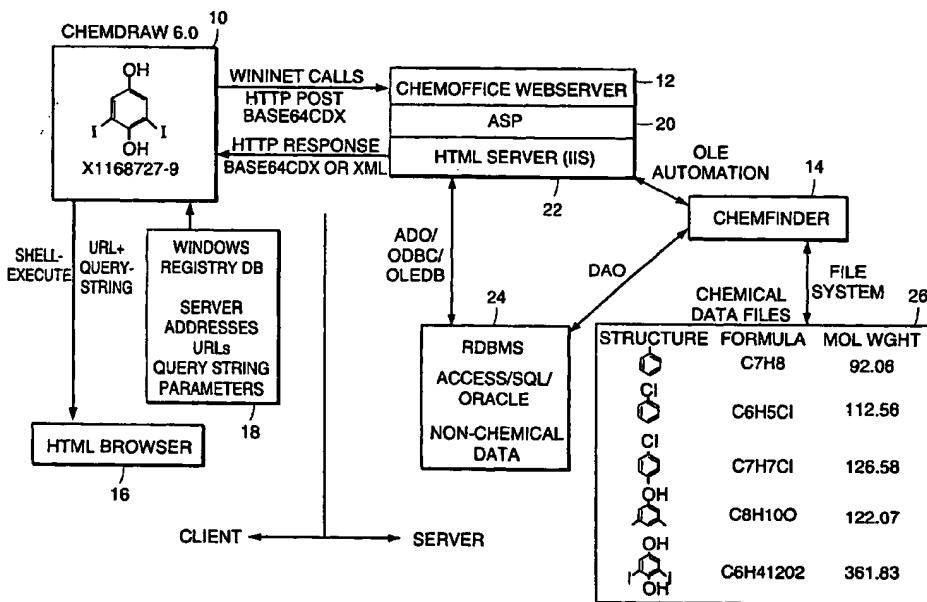
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(54) Title: MANAGING CHEMICAL INFORMATION AND COMMERCE



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(57) Abstract: A description of a chemical substance is acquired and a user's selection of a user interface menu item is detected. The user interface menu item pertains to a Web server having access to data for chemical substances. Based on the detection, a request is submitted to the Web server for information based on the description of the chemical substance. A response is received from the Web server that includes data pertaining to the chemical substance. Output data is derived from the data pertaining to the chemical substance.

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For two-letter codes and other abbreviations, refer to the "Guidance Notes on Codes and Abbreviations" appearing at the beginning of each regular issue of the PCT Gazette.

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see PCT Gazette No. 01/2003 of 3 January 2003, Section II

MANAGING CHEMICAL INFORMATION AND COMMERCE

This application claims the benefit of United States Provisional Application Serial No. 60/186,156 entitled "MANAGING CHEMICAL PRODUCT COMMERCE", filed on February 29, 2000, which is incorporated herein by reference.

5

Background of the Invention

This application relates to managing chemical information and commerce.

A chemistry oriented application program such as a chemical drawing program allows chemical information to be handled as computer data by a computer. A chemical drawing program typically allows a user to cause chemical structural information and chemical reaction information to be displayed on a computer screen and printed out on a computer printer. If a user has chemical information in the application program that is relevant to another application program, the user typically can use the cut and paste capabilities of the application program to copy the relevant information to the other application program. If one of the application programs is a Web browser interacting with a Web server, the user typically can use the cut and paste capabilities to share information between the Web browser and the other application program, and can thereby, in a limited way, share information between the Web server and the other application program. However, existing chemically oriented application programs provide inadequate abilities to access chemical information that is stored in different formats or in remote locations.

20

Summary of the Invention

Methods and systems are provided for managing chemical information and commerce. In particular, an external query capability allows a chemistry oriented application program to query an external entity such as a chemical information external database using

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the Hypertext Transfer Protocol ("HTTP"), to produce information management and commerce management results not otherwise realizable by the application program.

Different aspects of the invention allow one or more of the following. An application program having chemical information can submit that information in a query to a remote

- 5 chemical database and receive and incorporate a response from the database, without requiring the user to run or exercise another application program such as a Web browser. A user can provide chemical information in one form (e.g., structural) to an application program which can submit the information to another entity such as a remote database in a different form (e.g., textual) that is meaningful to the other entity, and that can lead to retrieval of
- 10 information that is useful to the user. The capabilities of a chemistry oriented software tool can be linked to, and thereby applied to, a remote organized set of chemical information to produce analytical and commercial results such as reports and purchasing lists based on the remote organized set of chemical information.

Other features and advantages will become apparent from the following description,

- 15 including the drawings, and from the claims.

Brief Description of the Drawings

Fig. 1 is a block diagram of a computer-based system.

Figs. 2-11, 16 are illustrations of output displays that may be produced by the computer based system.

- 20 Figs. 12A-15 are illustrations of data forms that may be used in the computer based system.

Detailed Description

A chemistry oriented application program has an external query capability that allows the program to query an external entity such as a chemical information external database.

Fig. 1 illustrates an example system in which a chemical drawing application program

- 5 10 (in this example, ChemDraw 6.0, provided by CambridgeSoft Corporation of Cambridge, Massachusetts) serves as the application program and uses the external query capability to acquire information via HTTP from a Web server 12 (in this example, ChemOffice WebServer, provided by CambridgeSoft Corporation of Cambridge, Massachusetts) linked to a chemical information database 14 (in this example, ChemFinder, provided by
- 10 CambridgeSoft Corporation of Cambridge, Massachusetts). Although these particular chemistry oriented programs are provided to illustrate the present invention, other applications programs, Web servers, databases, and other programs may be used as well or instead.

In the example system, which is a Microsoft Windows implementation using

- 15 ChemDraw, ChemDraw can, if necessary, invoke a Web browser 16 (e.g., see the third and fourth examples below) and can retrieve information including server addresses, uniform resource locators (URLs), and query string parameters from a Windows registry database ("Windows registry") 18. ChemDraw can use WinInet calls to post HTTP requests to the ChemOffice Webserver, and receives responses in HTTP form. WinInet, which is supplied as
- 20 part of the Windows operating system, is a set of functions (also known as calls, procedures, and subroutines) in an Internet application programming interface (API) that may be implemented as dynamic link library file (DLL). A DLL provides a library of functions that applications link to and call as regular function calls.

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The ChemOffice WebServer uses Active Server Pages ("ASP") software 20 and Hypertext Markup Language (HTML) server software known as Internet Information Server ("IIS") 22 to interact with ChemFinder via Object Linking and Embedding (OLE)

Automation, and with a relational database management system ("RDBMS") 24. (Other

- 5 interaction mechanisms may be used in place of or in addition to OLE Automation.) Web pages managed by ChemOffice WebServer may be formatted according to HTML or XML (Extensible Markup Language). Additionally, Web pages may be formatted as, for example, active server page text files ("ASP files") compatible with the ASP software. An ASP file may rely on a combination of HTML or XML and a scripting language such as VBScript or
- 10 JavaScript.

The interaction with the RDBMS is implemented using one or more data access technologies such as Open Database Connectivity (ODBC), Active Data Objects (ADO), and OLEDB. ODBC is a standard for accessing different database systems from a high level programming language application, and enables applications to submit statements to ODBC

- 15 using structured query language (SQL), which statements are then translated to the particular SQL commands that are used by the specific underlying database product.

- The RDBMS includes non-chemical data such as substance prices. ChemFinder is able to retrieve chemical information such as chemical structure data ("chemical structure"), chemical formulas, and molecular weights from chemical data files 26, and interacts with the
- 20 RDBMS using, e.g., ADO technology. According to ADO, data from a database is mapped into active data objects which perform the actual queries to the database. This approach provides substantial abstraction by limiting exposure only to the resultant objects.

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ChemDraw communicates with an external chemical database server as now described with reference to multiple examples including an example illustrating how ChemDraw may be used to purchase chemicals online at the Available Chemicals Xchange web site (ChemACX.com). ChemDraw can initiate a database query based on either a

5 chemical structure drawing or a simple text string. (Other application programs may use other data formats.) The response provided by the chemical database server can be a simple text response, a chemical structure, or a complex record set containing a combination of chemical and non-chemical data. The process by which ChemDraw handles a query differs slightly depending on the request/response method that is available.

10 In a first example, a chemical structure drawing is used to retrieve a plain text response. Using ChemDraw, the user creates a drawing of a molecule which is stored as chemical structure by ChemDraw in a native binary format known as cdx.

When the user selects "Look up ACX number from structure" from an online menu
40 (Figs. 2-3), which is a pulldown menu in ChemDraw, ChemDraw converts the chemical
15 structure data from the cdx format to an ASCII text representation. The cdx-to-ASCII conversion is accomplished via a base64 encoding process with a subsequent URL encoding for safe transport over the HTTP protocol. Base64 is an encoding scheme defined by the Multipurpose Internet Mail Extensions (MIME) standard, and is defined to provide robustness to binary data that is expected to confront transformations while traversing the
20 Internet. Base64 encoding converts binary data into alphanumeric characters. For example, binary data such as "110110001011010100000101" may be encoded as textual data "sLUF" which may be transmitted across the Internet.

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ChemDraw uses configuration information stored in the Windows registry database to derive a target URL, i.e., a URL pointing to a remote chemical database server. Using the URL derived from the registry information and the URL encoded ASCII text representation of the chemical structure drawn by the user, ChemDraw uses WinInet to post an HTTP request.

5 The converted chemical structure data is passed in the body of the HTTP request.

The remote chemical database server responds with a comma delimited text string containing one or more ACX numbers (e.g., ACX number X1069636-5 shown in Fig. 4) corresponding to the chemical structure drawn by the user. (ACX numbers are product identifiers described in two commonly assigned co-pending applications filed May 5, 2000:

10 09/565,085 entitled "DERIVING PRODUCT INFORMATION", and 09/565,810 entitled "MANAGING PRODUCT INFORMATION", which applications are incorporated herein by reference.)

ChemDraw captures the server's response by reading the HTTP response.

As shown by example in Fig. 5, the ACX numbers received from the server are

15 displayed by ChemDraw on the ChemDraw canvas in a text box displayed near, e.g., immediately below, the user's chemical structure drawing.

In a second example, a plain text input value is used to retrieve a chemical structure drawing. In particular, a reverse version of the first example above can be accomplished by providing a valid ACX number and retrieving the corresponding chemical structure. In this 20 example, the user selects "Lookup structure from the ACX number" in the ChemDraw 6.0 online menu.

A dialog box shown by example in Fig. 6 opens and prompts the user to enter an ACX number.

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ChemDraw retrieves target URL information from the Windows registry and builds an HTTP request. In this case, the payload of the HTTP request is a string containing the ACX number, which is appended to the URL as a query string. The HTTP response returned by the remote server contains a URL encoded base64 text representation of a chemical structure. ChemDraw decodes the text representation and displays the structure on its canvas as a native ChemDraw picture shown by example in Fig. 7.

In a third example, an external HTML browser session is initiated with a remote server. Although ChemDraw is able to access remote servers by directly managing HTTP calls, ChemDraw can also delegate interactions with the server to an external HTML browser. A user selects a “Browse ChemStore.Com” online menu item in ChemDraw, which causes the default HTML browser to be launched on the user’s computer and directed to load a Web page from ChemStore.com as shown by example in Fig. 8.

ChemDraw proceeds in the third example as follows. ChemDraw builds a URL from configurable data stored in the Windows registry. ChemDraw issues a call to ShellExecute with the target URL as a parameter, which causes the user’s default browser to open and load the page specified by the URL. (In Microsoft Windows, the ShellExecute function either launches the specified application program, or, if the program is already executing, makes the program the current window.)

Complex URLs corresponding to user specific server pages can be built by incorporating data received from previous queries using techniques described in the first and second examples above. For example, a specific page from a chemical supplier’s catalog can be retrieved based on a structure of a molecule drawn by the user.

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In a fourth example, a user accomplishes online purchasing of chemicals by starting from ChemDraw. The first and second examples above illustrate how ChemDraw can send or receive a chemical structure or text data to or from a remote chemical database server and display the results directly in ChemDraw's drawing area. When the results of a query are 5 expected to be lengthy or complex, ChemDraw causes a standard HTML browser to handle the display instead.

In this example, chemicals are purchased online from ChemACX.com. As described in the first example above, the user draws a molecule and selects the "Lookup suppliers from ChemACX.com" online menu item.

10 The chemical structure drawn by the user is used in this example to identify the substance for which purchasing information is to be fetched. Thus, the procedure is as described in the first example above, except that the value returned by the server is a substance identifier that is not meaningful to the end user, and therefore is not displayed, but is used as an intermediate value for querying a Web based catalog.

15 Specifically, the substance identifier is posted to a remote server to obtain the desired purchasing information. The requested result set is to be displayed in an external browser window. Accordingly, ChemDraw uses techniques described above in the third example to build a URL pointing the specific catalog page at ChemACX.Com which contains information about the desired substance. This URL is built from server target information 20 stored in the Windows registry database and from the unique substance identifier fetched from the server in the initial step described above.

ChemDraw opens the user's default external browser and automatically causes the browser to load the appropriate catalog page. The user can use the browser to navigate the

available purchasing information and initiate the online ordering process from within the browser.

In a specific implementation in which the user is presented with a list of suppliers and prices in a Web browser window, the user can then check off the supplier and desired
5 quantity, which causes a corresponding shopping cart construct to be created, ready for submission for purchase completion.

The online menu may also be configured to retrieve other pieces of data based on a selected structure, such as specific compound identification numbers from specific manufacturers.

10 Figs. 12A-16 illustrate a specific example of data transformations referenced above, with respect to an example interaction when a user draws a structure and selects the "Find ACX Numbers from Structure" online menu item. Figs. 12A-12B illustrate a chemical structure and its corresponding binary CDX form. Fig. 13 illustrates the base64 encoded form corresponding to Figs. 12A-12B. Fig. 14 illustrates the encoded request corresponding
15 to Fig. 13. Fig. 15 illustrates the response from the server corresponding to Fig. 14. Fig. 16 illustrates a display provided to the user corresponding to Fig. 15.

Figs. 9-11 illustrate examples of other pages that may be retrieved by selection of, respectively, the "CambridgeSoft Home Page", "CS ChemDraw Technical Support", and "Register Online" online menu items shown in Figs. 2-3.

20 All, or a portion, of the procedures described above may be implemented in hardware or software, or a combination of both. In at least some cases, it is advantageous if the technique is implemented in computer programs executing on one or more programmable computers, such as a personal computer running or able to run an operating system such as

- 10 -

Unix, Linux, Microsoft Windows 95, 98, 2000, or NT, or Macintosh OS, that each include a processor, a storage medium readable by the processor (including volatile and non-volatile memory and/or storage elements), at least one input device such as a keyboard, and at least one output device. Program code is applied to data entered using the input device to perform

5 the technique described above and to generate output information. The output information is applied to one or more output devices such as a display screen of the computer.

In at least some cases, it is advantageous if each program is implemented in a high level procedural or object-oriented programming language such as Perl, C, C++, or Java to communicate with a computer system. However, the programs can be implemented in

10 assembly or machine language, if desired. In any case, the language may be a compiled or interpreted language.

In at least some cases, it is advantageous if each such computer program is stored on a storage medium or device, such as ROM or optical or magnetic disc, that is readable by a general or special purpose programmable computer for configuring and operating the

15 computer when the storage medium or device is read by the computer to perform the procedures described in this document. The system may also be considered to be implemented as a computer-readable storage medium, configured with a computer program, where the storage medium so configured causes a computer to operate in a specific and predefined manner.

20 Other embodiments are within the scope of the following claims. For example, a more general range of services may be provided. A query may be performed on local or remote databases, and may be used in the derivation of a non-exact query or a non-structural query. For instance, in the case of ChemDraw which provides property prediction facilities,

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such facilities may be used to predict physical characteristics of a molecule of interest, and local or remote databases may be searched for substances having similar properties. The online menu may be used in another application program such as a spreadsheet program. For instance, in the case of the spreadsheet program, the program may store a shopping list of 5 chemical products, and the online menu may include a selectable item for retrieving price information for each listed product from a remote chemical information database and embedding the retrieved price information in the shopping list.

What is claimed is:

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1. A method for use in managing chemical information, comprising:
acquiring a description of a chemical substance;
detecting a user's selection of a user interface menu item pertaining to a Web server
having access to data for chemical substances;
- 5 based on the detection, submitting, to the Web server, a request for information based
on the description of the chemical substance;
receiving a response from the Web server, the response including data pertaining to
the chemical substance; and
deriving output data from the data pertaining to the chemical substance.
- 10 2. The method of claim 1, wherein the description of the chemical substance includes
a structural description of the chemical substance.
- 15 3. The method of claim 1, wherein the description of the chemical substance includes
a textual description of the textual substance.
- 20 4. The method of claim 1, wherein the output data includes structural output data.
5. The method of claim 1, wherein the output data includes textual output data.

6. The method of claim 1, wherein the output data includes commercial product data.
7. The method of claim 1, wherein the user interface item is provided by a chemistry
oriented application program.

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8. The method of claim 7, wherein the chemistry oriented application program includes a chemical drawing program.

9. The method of claim 1, further comprising

5 formatting at least a portion of the request for information according to the HTTP protocol.

10. The method of claim 1, further comprising

decoding at least a portion of the response from the Web server according to the

10 HTTP protocol.

11. The method of claim 1, further comprising

presenting a user interface window that includes a display corresponding to the description of the chemical substance and another display derived from the output data.

15

12. The method of claim 1, further comprising

causing a new Web browser window to be displayed; and

causing a display derived from the output data to be displayed in the new Web browser window.

20

13. Computer software, residing on a computer-readable storage medium, comprising a set of instructions for use in a computer system to help cause the computer system to manage chemical information, the instructions causing the system to:

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- acquire a description of a chemical substance;
- detect a user's selection of a user interface menu item pertaining to a Web server having access to data for chemical substances;
- based on the detection, submit, to the Web server, a request for information based on 5 the description of the chemical substance;
- receive a response from the Web server, the response including data pertaining to the chemical substance; and
- derive output data from the data pertaining to the chemical substance.

- 10 14. A system for use in managing chemical information, comprising:
- a Web server having access to data for chemical substances; and
 - a chemistry oriented application program providing a user interface menu item linked to the Web server.

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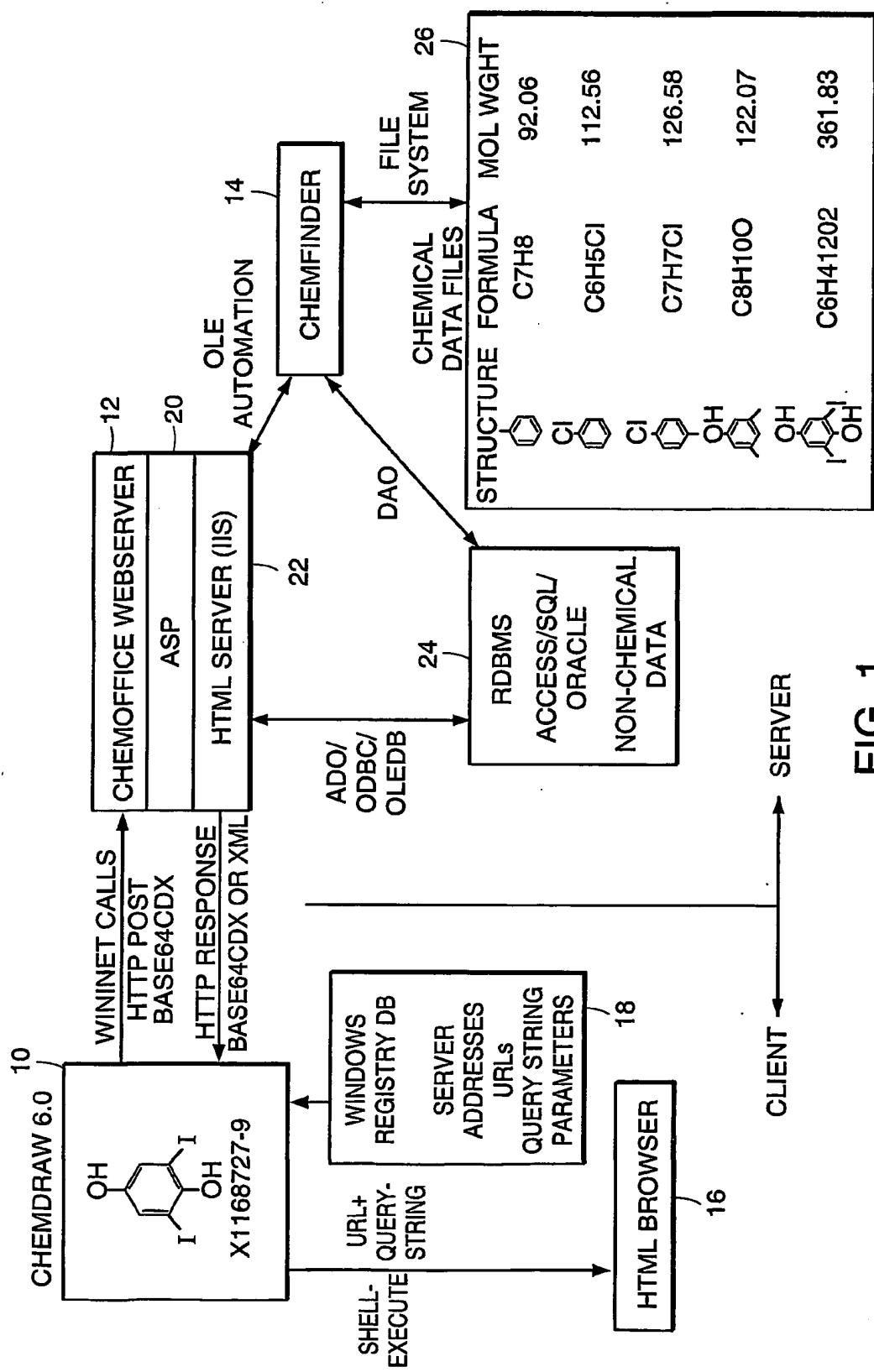


FIG. 1

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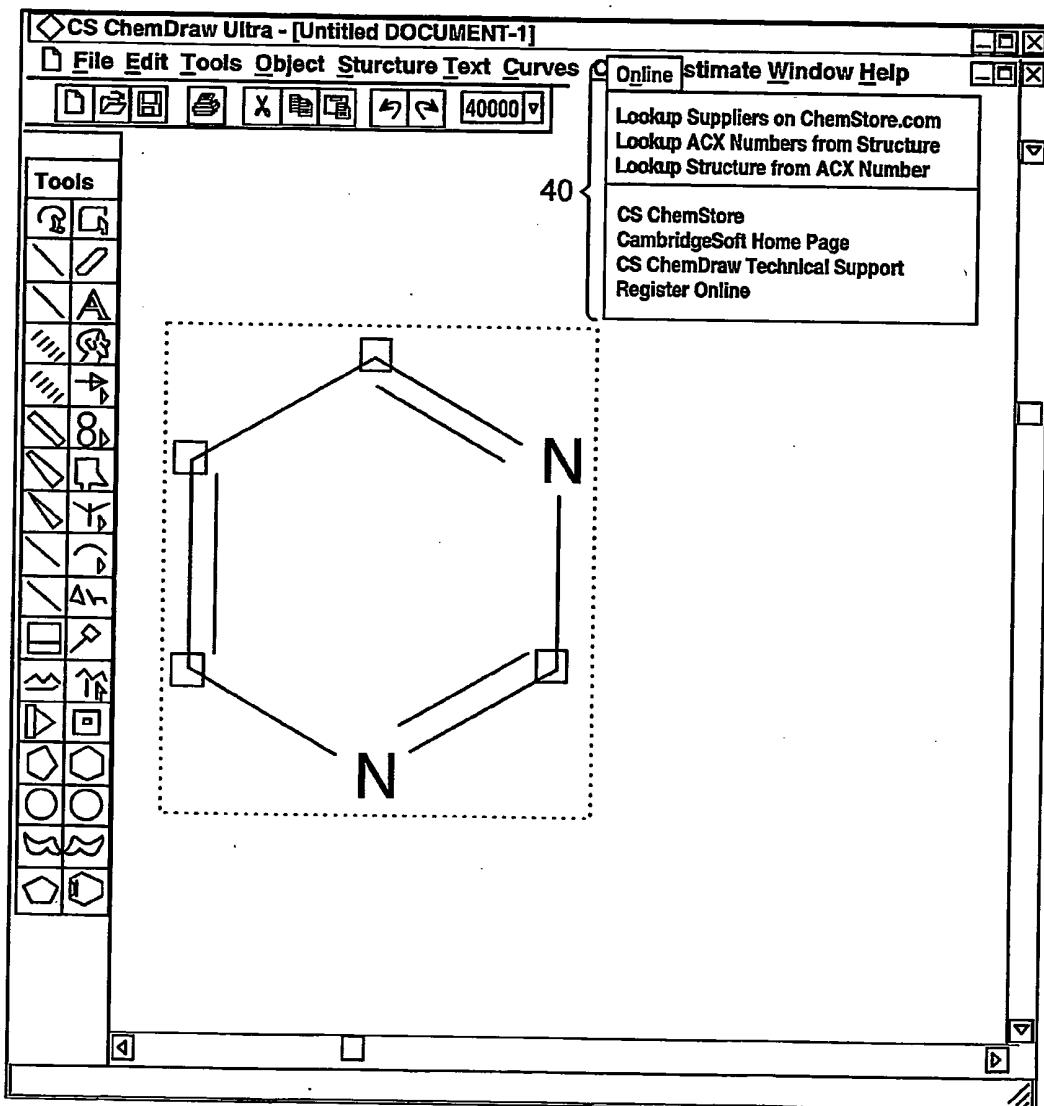


FIG. 2

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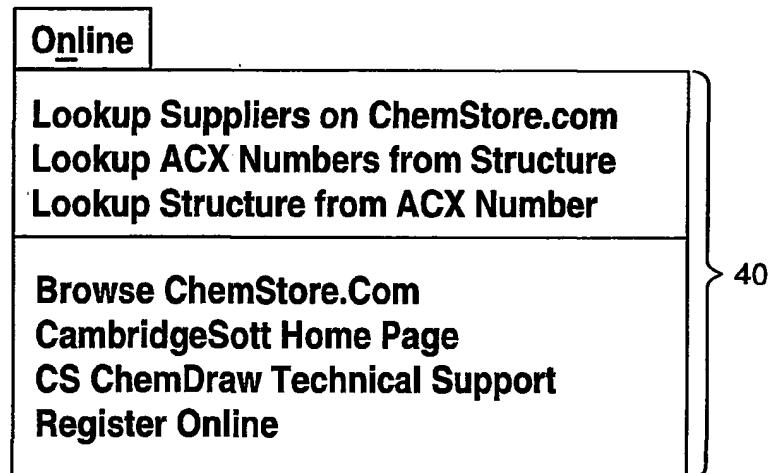


FIG. 3

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ChemOffice WebServer Substance List View

Total Records 176007

Comments

Internet Searching and Information

Prefences Help About Log Off

New Query Edit Query Refine Save Query Export Hits

Record 1-2 of 2 hits

View Clear

Record 1 of 2

Benzene-13C6 CAS Reg#: 32488-44-1

Formula: C₆H₆
MW: 78.1134
ACX Number: X10096365
of Suppliers: 2
of Products: 2

Mark Record Show Details

Record 2 of 2

FIG. 4

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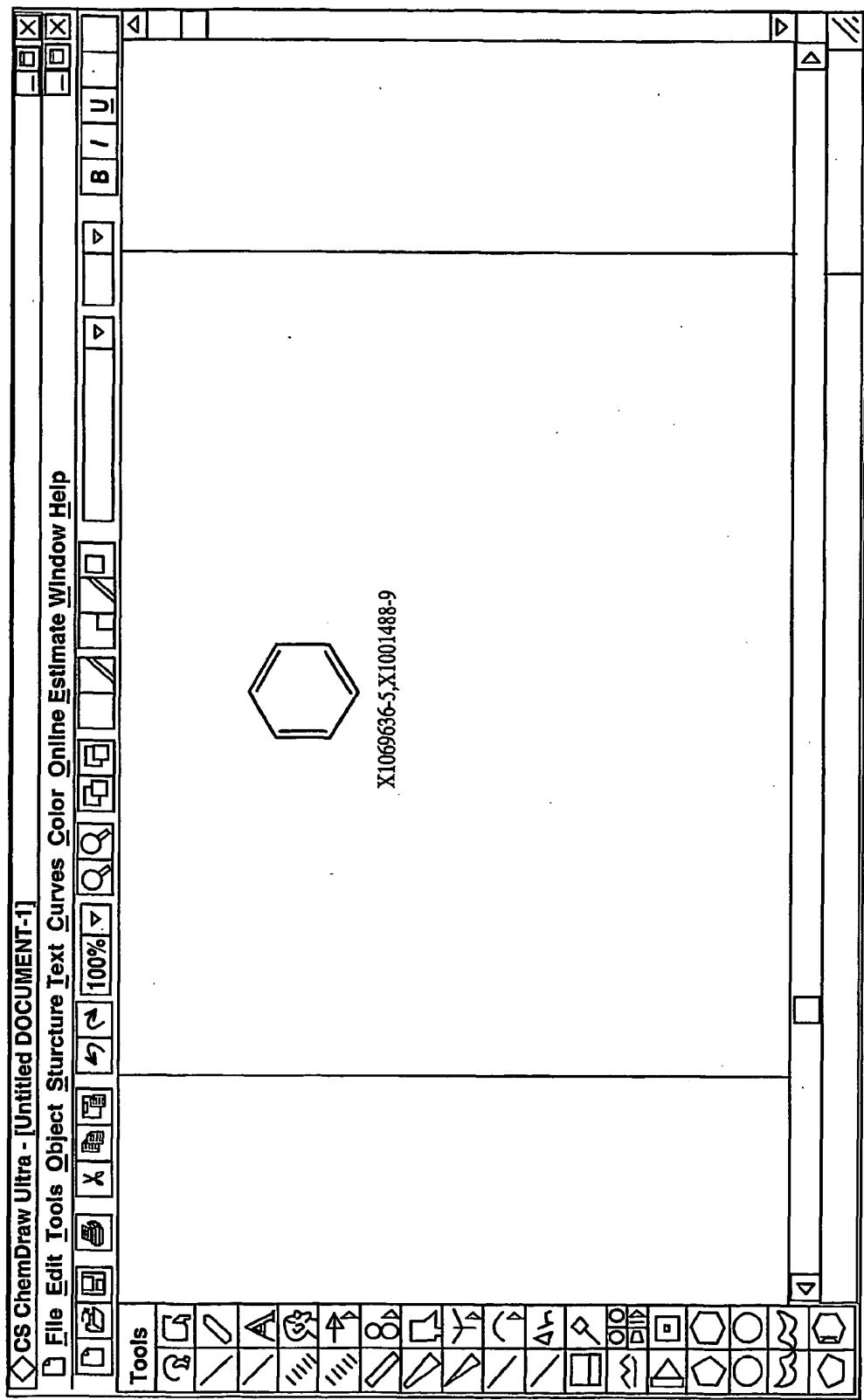


FIG. 5

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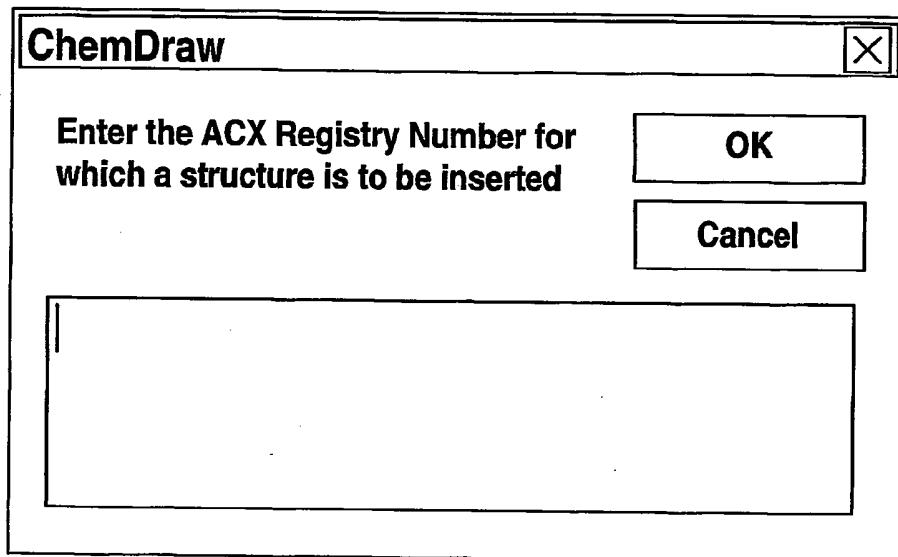


FIG. 6

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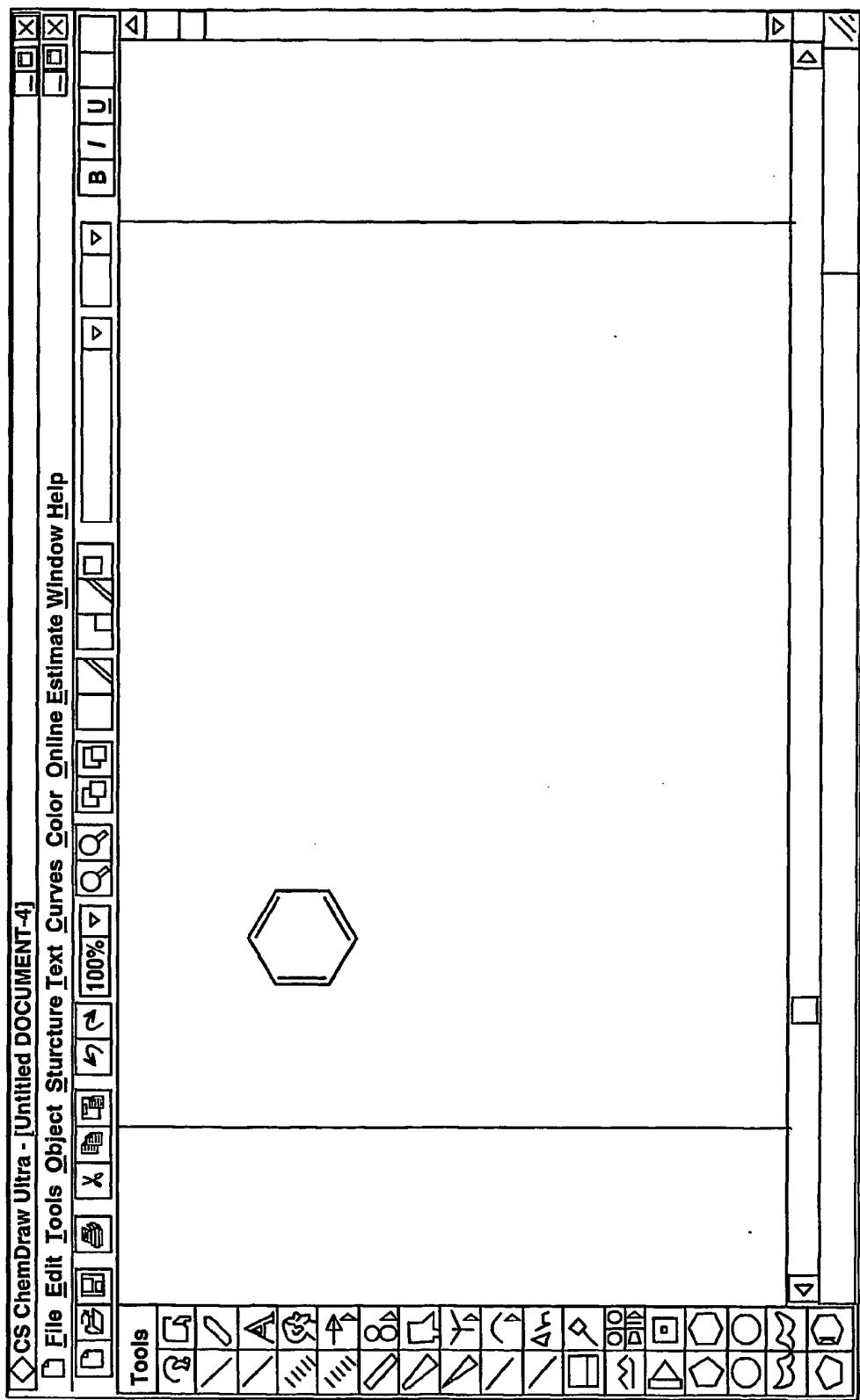


FIG. 7

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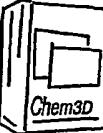
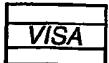
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<p>Visit our Virtual TradeShow! Booth Directory:</p> <p>ChemStore.Com now has five different departments to serve all your scientific software and chemistry needs!</p> <p>February ChemStore.Com Specials</p>				
<p>SciStore.Com</p> <p>Chem3D Ultra 5.0 - w/Chili Pepper SciOSAR 3.0</p> <p>ChemShirt</p>  <p>Powerful molecular modeling package with CS MOPAC, Gaussian interface, MM2 and Chem3D plugin for Windows and Macintosh</p> <p>Order today and receive a free <u>XL red Chili Pepper shirt!</u> List Price: \$995 SAVE \$200! Special prices: \$799-Eduprice: \$349</p> <p>ChemQuote.Com</p> <p>FREE  T-Shirt with order</p> <p>is for overstocked or large quantities of products or new or used equipment available for sale. Sort through our many listings for savings or post your items for sale. With your first purchase, get a FREE ChemShirt!</p> <p>ChemACX.Com</p>  <p>For a limited time, you can evaluate for FREE our ChemACX e-commerce chemical purchasing system, included with ChemOffice WebServer. Contact us at chemacx@camsoft.com for more details.</p> <p>ChemFinder.Com</p>  <p>Get a FREE 30 day trial subscription to ChemInfo Pro, the professional version of ChemFinder.Com subscription package. ChemInfo Pro features ChemACX Pro, ChemRXN Pro and ChemINDEX Std databases.</p>	<p>SciStore.Com</p> <p>Create Quantitative Structure-Activity or Property Relationships (QSAR/QSPR) to explain the observed activities or properties of compounds then predict them for new compounds.</p> <p>List Price: \$1295 SAVE \$300! Special prices: \$999-Eduprice: \$549</p> <p>LabEqwip.Com</p> <p>Join the LabEqwip Frequent Buyers Program</p> <p>Receive a 5% discount off of our already discounted prices when you make 5 or more purchases per month at LabEqwip. For more information please email labeqwip@camsoft.com.</p>			
	  			
<p>We accept Visa, MasterCard, and American Express for completely automated, secure, convenient ordering. We are also pleased to accept faxed purchase orders for orders totalling \$500 or more.</p>				
<p>ChemQuote.Com ChemACX.Com SciStore.Com LabEqwip.Com ChemSell.Com</p> <p>CambridgeSoft ChemFinder.Com ChemStore.Com ChemNews.Com ChemClub.Com</p>				

FIG. 8

SUBSTITUTE SHEET (RULE 26)

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 <p>ChemFinder ChemStore ChemNews ChemClub CambridgeSoft</p> <p>FREE!</p> <p>Products WebServer ChemOffice ChemDraw Chem3D ChemFinder ChemInfo Reviews</p> <p>Solutions</p> <p>E-Commerce E-Lab Book ComboChem Databases Registration Inventory Web Apps Oracle Reviews</p> <p>Purchase</p> <p>ChemStore Resellers More Info</p> <p>Cambridge Soft TechSupport Y2KSupport BetaTesting Jobs at CS Press Releases AboutCS Partners Contacts</p> <p>Languages</p> <p>Japenese Deutsch Francals</p> <p>ChemFinder ChemStore ChemNews ChemClub CambridgeSoft</p>	<table border="0" style="width: 100%; border-collapse: collapse;"> <tr> <td style="width: 20%;">CambridgeSoft</td> <td style="width: 20%;">ChemFinder.Com</td> <td style="width: 20%;">ChemStore.Com</td> <td style="width: 20%;">ChemNews.Com</td> <td style="width: 20%;">ChemClub.Com</td> </tr> <tr> <td>ChemQuote.Com</td> <td>ChemACX.Com</td> <td>SciStore.Com</td> <td>LabEqwip.Com</td> <td>ChemSell.Com</td> </tr> </table> <div style="text-align: center; margin-bottom: 10px;">  Chemistry, Community, Content & Commerce </div> <div style="text-align: center; margin-bottom: 10px;">  ChemNews.Com NEWS </div> <div style="text-align: right; border: 1px solid black; padding: 2px; margin-bottom: 10px;">  SOFTWARE </div> <h2>ChemNews.Com 10.1</h2> <p>Four Languages ENGLISH*FRANCAIS*DEUTSCH*日本語</p> <div style="display: flex; justify-content: space-between;"> <div style="width: 45%;"> <p> February 18, 2000 - Issue 10.1 of ChemNews.Com is online in four languages!</p> <p>The latest issue of ChemNews.Com is available online in English, French, German, and Japanese. Read a preview of ChemDraw 6.0, a review of chemistry textbooks, the latest in purchasing chemicals online, and more.</p> <hr style="margin: 10px 0;"/> <p> January 28, 2000 - LabEqwip.Com is open for business!</p> <p>LabEqwip.Com has laboratory instruments, equipment, and supplies available for sale. Search by keyword or category for the supplies you need.</p> <hr style="margin: 10px 0;"/> <p> January 7, 2000 - ChemOffice WebServer 2000 is now available for you to purchase!</p> <p>ChemOffice WebServer 2000 is available in both Ultra and Pro versions. It is the latest version of the remarkable ChemOffice WebServer software, capable of delivering chemical information and databases to the desktop machines throughout your office.</p> <hr style="margin: 10px 0;"/> <p><i>CambridgeSoft.Com develops, markets and supports high quality Internet software applications for chemists and engineers.</i></p> </div> <div style="width: 45%;"> <p>Talk to CambridgeSoft.Com</p> <p>Have one of our representatives contact you by phone to answer your questions.</p> <p> CALL ME NOW</p> <p>Free Downloads</p> <p>Download free software at FreeChem.Com</p> <p>Free CD-ROM</p> <p>Receive Product Literature and a Free CD-ROM by mail. The CD contains software, including ChemOffice Net and the ChemOffice Net Plugins, as well as demos, multimedia, and issue of ChemNews.Com</p> <p>Buy Online</p> <p>Shop for software, computers, books, t-shirts, and more at SciStore.Com. Buy chemicals at ChemACX.Com. Buy lab equipment, instruments, and supplies at LabEqwip.Com. Buy products on auction sale at ChemSell.Com. Request for product quotations at ChemQuote.Com.</p> </div> </div>	CambridgeSoft	ChemFinder.Com	ChemStore.Com	ChemNews.Com	ChemClub.Com	ChemQuote.Com	ChemACX.Com	SciStore.Com	LabEqwip.Com	ChemSell.Com
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FIG. 9

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FIG. 10

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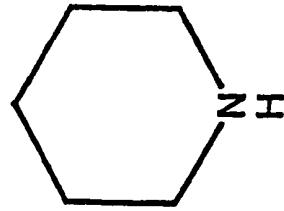
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FIG. 11
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FIG. 12A-1
FIG. 12A-2
FIG. 12A-3

FIG. 12A



01983569 56 6A 43 44 30 31 30 30 04 03 02 01 00 00 00 00
01983579 00 00 00 00 00 00 00 00 00 00 00 00 00 03 00 12 00
01983589 00 00 43 68 65 6D 44 72 61 77 20 36 2E 30 2E 33 .ChemDraw 6.0.3

FIG. 12A-1

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01983599	62	39	08	00	15	00	00	55	6E	74	69	74	6C	65	64	b9.....Untitled Document -1..2..	
019835A9	20	44	6F	63	75	6D	65	6E	74	2D	31	00	03	32	00	08	.YyYyyY.. Y.Y..
019835B9	00	FF	00	00	00	00	FF	FF	00	.YyYyyY.. Y.Y..							
019835C9	00	00	FF	00	00	00	00	FF	FF	00	.YyYyyY.. Y.Y..						
019835D9	00	FF	00	00	00	00	FF	FF	00	.YyYyyY.. Y.Y..							
019835E9	FF	00	09	00	00	01	09	08	00	00	00	00	68	00	00	96	.YyYyyY.. Y.Y..
019835F9	00	02	09	08	00	00	00	4D	02	00	00	3B	03	02	08	10	.YyYyyY.. Y.Y..
01983609	00	00	00	24	00	00	00	24	00	00	00	24	00	00	00	24	.YyYyyY.. Y.Y..
01983619	00	03	08	04	00	00	00	78	00	04	08	02	00	78	00	05	.YyYyyY.. Y.Y..
01983629	08	04	00	00	00	1E	00	06	08	04	00	00	00	04	00	07	.YyYyyY.. Y.Y..
01983639	08	04	00	00	00	01	00	08	08	04	00	00	00	02	00	09	.YyYyyY.. Y.Y..
01983649	08	04	00	33	B3	02	00	0A	08	08	00	03	00	60	00	C8	.YyYyyY.. Y.Y..
01983659	00	03	00	0B	08	08	00	04	00	00	00	F0	00	03	00	0D	.YyYyyY.. Y.Y..
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01983679	00	00	00	19	D	13	57	FF	A9	FF	B2	19	71	13	9E	03	.YyYyyY.. Y.Y..
01983689	67	05	28	03	FC	00	02	00	00	02	58	02	58	00	00	00	.YyYyyY.. Y.Y..
01983699	00	19	0D	13	57	00	01	00	64	00	64	00	00	00	01	00	.YyYyyY.. Y.Y..
019836A9	01	01	01	00	00	00	01	27	0F	00	01	00	01	00	00	00	.YyYyyY.. Y.Y..
019836B9	00	00	00	00	00	00	00	00	00	00	02	00	19	01	90	00	.YyYyyY.. Y.Y..
019836C9	00	00	00	00	60	00	00	00	00	00	00	00	00	01	00	00	.YyYyyY.. Y.Y..

FIG. 12A-2

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FIG. 12A-3

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FIG. 12B

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FIG. 13

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FIG. 14

FIG. 14A
FIG. 14B

POST HTTP/1.1
/chemacx/chemacx_chemacx_action.asp?dbname=chemacx&dataaction=search_no_gui
Accept: */*
Host: chemdraw.chemacx.com
Referer: Online
User-Agent: CS ChemDraw Ultra 6.0
Cookie: ASPSESSIONIDGGGGRID=BELBBHJCLDCFHMMOPNDDKFLBO
Content-Length: 1481
Content-Type: application/x-www-form-urlencoded
Cache-Control: no-cache

FIG. 14A

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```

return_fields=Substance.ACX_ID&struc_search_type=exact&Substance.Structure=
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YjklABUAAAABVbnRpDGx1ZCBeB2N1bwVudCOxAmYAAGA// //// /AAAAAAA/ /8A
AAAA// // /wAAAAD/ /wAAAAD// // /AAAAAP// // /AAKMAAEJCAAAGGAAACTW
AAIJCAAAAE0CAA7AWIIEAAAACQAAAACKAAAJJAAAACQQAAGWEAAAECAlaeAAF
CAQAAAACeAYIBAAAQQABwGEAAAQQAIICAQAAAACAkIBAAZSWIACGGIAAMAYADI
AAMACWgIAAQAAAADWAAAMADQ9AAAJeAAAIAAAA19CWAAAQAZDRNX/6n/shlXe54D
ZwUOA/wAAGAAA19CWAAAQAZDRNKAEEAZABKAQAAAQABAQEAAAABJw8AAQABAAA
AAAAAAABeAAAAvQAAK4AAAD6AAABJAAAIAAwdkBAUQAQXJPyWWEAQEDWBHUaw1
CYBOZXCgUm9tYW4BqA4AAAEEhAAAABeAAAAvQAAK4AAAD6AA8IAGABABALAGAB
ABYIBAAAACQAGAGEAAA4PAAA4PAAA4PAAA4PAAA4PAAA4PAAA4PAAA4PAAA
gAEAAAAKAAIAQAAAGAAAABxAOWeWQAA3BAEAAAQABIAZCAAACGACAAIAAAIAAAA
jwDSBMEANwQBAEAAAASAAWAAAQAAAGADAACCCAAAQAAQAAQAAQAAQAAQAAQAAQAAQ
AAAHdgABAQAAAwBqAMgAAwBOSAQHb9ACAAIAAWAFBWEABQACCABm5QEADDYAAQC
EAQAAJSAADZAAAIAAAAN4AAA3BAEAAQITEAqAHACSEAGABAABIAEAAAHEAE/v0ADCE
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BAYEAAEAAAEGFB9QAAQAAQGAAQBAAAAFgqAGAAAQAAKAIAACAAEB9QAAQAAUGBAAD
AAAACgYBAEAAAAWACQAAAQGJAAQGBRAADAAAABQYEAAQAAAKB9EAAQAABYAK
AAAACgACAAQABAYEAAQAAAQAAAQFB9QABQAAAOCQABAAAQfQASAAAQAAKAIA
BQAAAUGBAAGAAAACgYBAEAAAQWADAAAQgAMAQGBAAGAAAABQYEAAEAAA
B9EAAQAAA

```

FIG. 14B

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HTTP/1.1 200 OK
Server: Microsoft-IIS/4.0
Date: Wed, 28 Feb 2001 17:34:38 GMT
Content-Type: text/html
Cache-control: private
Transfer-Encoding: chunked

X1001495-4

FIG. 15

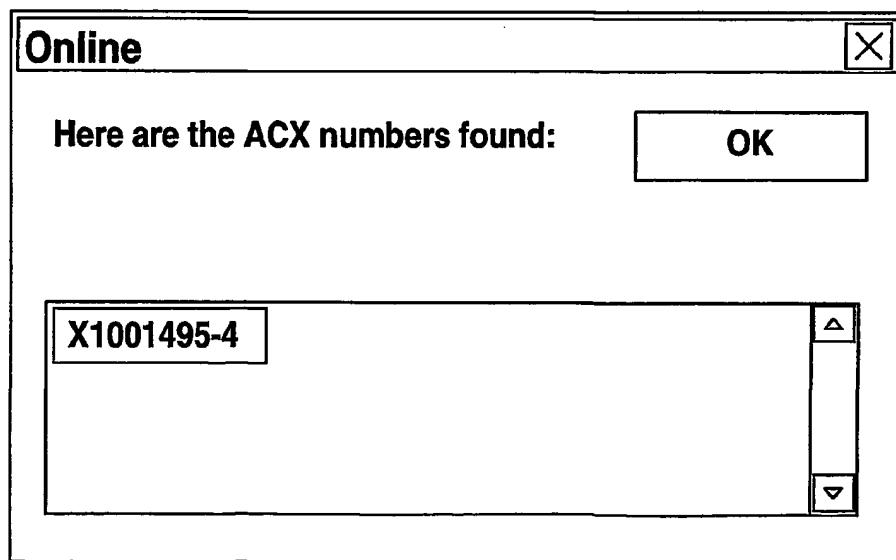


FIG. 16

INTERNATIONAL SEARCH REPORT

International application No
PCT/US 01/06443

A. CLASSIFICATION OF SUBJECT MATTER
IPC 7 G06F17/30

According to International Patent Classification (IPC) or to both national classification and IPC

B. FIELDS SEARCHED

Minimum documentation searched (classification system followed by classification symbols)
IPC 7 G06F

Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched

Electronic data base consulted during the international search (name of data base and, where practical, search terms used)

EPO-Internal, WPI Data, PAJ, INSPEC, COMPENDEX, IBM-TDB

C. DOCUMENTS CONSIDERED TO BE RELEVANT

Category	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
X	IHLENFELDT W-D ET AL: "BEYOND THE HYPERACTIVE MOLECULE: SEARCH, SALVAGE AND VISUALIZATION OF CHEMICAL INFORMATION FROM THE INTERNET" PACIFIC SYMPOSIUM ON BIocomputing '96. HAWAII, JAN. 3 - 6, 1996, SINGAPORE, WORLD SCIENTIFIC, SI, vol. SYMP. 1, 3 January 1996 (1996-01-03), pages 384-395, XP000751937 ISBN: 981-02-2578-4 section 4: Application Examples figures 1-5 -/-	1-14

Further documents are listed in the continuation of box C.

Patent family members are listed in annex.

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04/07/2002

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INTERNATIONAL SEARCH REPORT

International Application No
PCT/US 01/06443

C(Continuation) DOCUMENTS CONSIDERED TO BE RELEVANT

Category	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
X	ERTL P ET AL: "WWW-BASED CHEMICAL INFORMATION SYSTEM" JOURNAL OF MOLECULAR STRUCTURE (THEOCHEM), ELSEVIER SCIENCE PUBLISHERS B.V., AMSTERDAM, NL, vol. 419, 8 December 1997 (1997-12-08), pages 113-120, XP000957419 ISSN: 0166-1280 Section 1: Introduction figures 1-7 --- 	1-14
A	US 5 978 804 A (DIETZMAN GREGG R) 2 November 1999 (1999-11-02) column 2, line 64 -column 3, line 67 --- 	1,13,14
A	US 6 023 659 A (AKERBLOM INGRID E ET AL) 8 February 2000 (2000-02-08) column 2, line 16 -column 4, line 20 --- 	1,13,14

INTERNATIONAL SEARCH REPORT

Information on patent family members

International application No
PCT/US 01/06443

Patent document cited in search report	Publication date	Patent family member(s)		Publication date
US 5978804	A 02-11-1999	NONE		
US 6023659	A 08-02-2000	US	6363399 B1	26-03-2002
		US	5953727 A	14-09-1999
		US	6189013 B1	13-02-2001